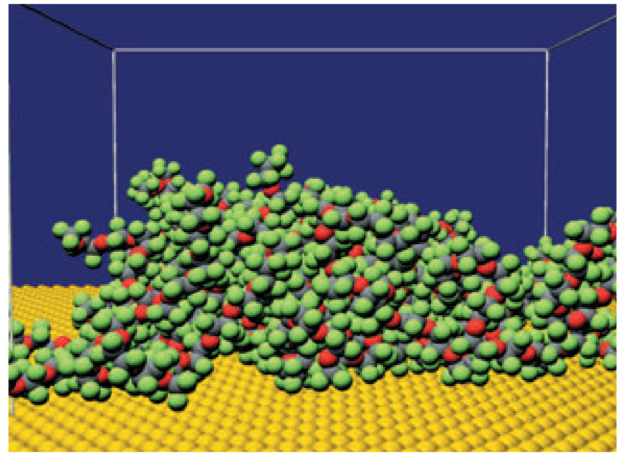
Using Computers to Build Better Computers



Lubricant PFPE

COMPUTER hard drives on the market today can store 578 megabits of data per square inch of disk surface area. Even greater storage capacity is on the horizon. One gigabit (1 billion bits) per square inch of magnetic disk has already been demonstrated in the laboratory, and the fundamental limit of storage for magnetic technology is on the order of 100 billion bits per square inch of data.

Three issues are central to increasing the storage capacity of magnetic hard drives. The first is decreasing the size of the magnetic domain that stores a bit of information. The second is creating a read/write head capable of sensing the very weak fields from the smaller domains. The third is moving the head closer to the surface of a spinning disk without introducing deleterious friction and wear.

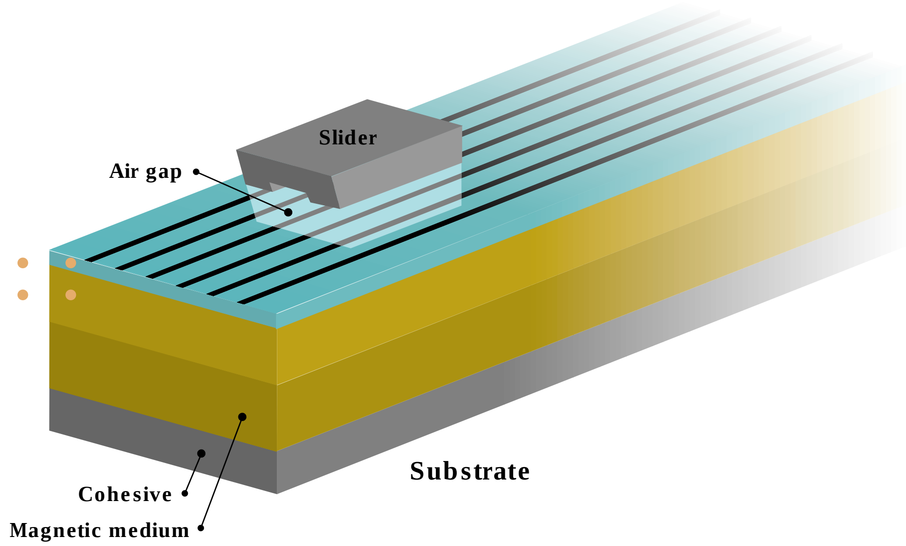
Last year, the Laboratory and IBM's Almaden Research Center in San Jose, California, signed a cooperative research and development agreement (CRADA) to study the relevant friction and wear mechanisms. The three-year agreement is valued at $1.6 million with costs shared equally by the two partners. The next-generation, super-high-capacity, hard-disk drives will increase the disk-storage capacity tenfold, to about 10 gigabits of data per square inch.

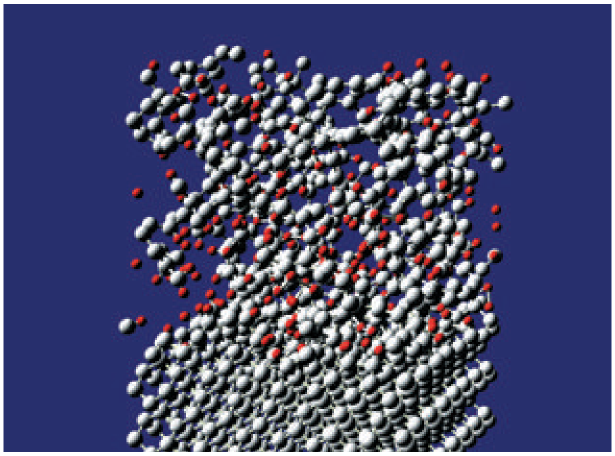
The fundamental problem associated with minimizing friction and wear mechanisms is to gain a better understanding of the underlying chemical and physical processes at the point where a disk drive's read/write head skims closest to the surface of a spinning hard disk (see figure). The interactions at this interface take place at such high speeds and short distances that atomic-level computer simulation may be the only way to envision the details of what may be happening there. Here is a case where modern computers can be applied to build even better computers. In more technical terms, this is a problem where the Laboratory's expertise in atomistic molecular dynamics (MD) modeling is being put to practical use in advancing data-storage technology itself. (The article on p. 13 gives more details on how MD modeling is used to study tribological—that is, friction and wear—processes.)

As shown in the figure, today's disk drives have a gap of only about 75 nanometers (3 millionths of an inch) between the slider, which carries the read/write head, and the disk surface. The disk also rotates very rapidly, between 3600 and 7200 rpm. Thus, the outer edge of the disk travels between 12 and 24 m/s with respect to the slider. These dimensions and velocities make the problem an ideal one for MD computer simulation. The entire slider–disk interface problem can be modeled using about 100 million atoms, which fits in the main memory available on a modern parallel supercomputer. One tool that Laboratory scientists use to analyze the enormous amount of information from these simulations is computer animation. The animated movies show the behavior of individual atoms and molecules at the slider–disk interface.

Between the magnetic substrate and the flying head is a thin coating (30 nm) of amorphous hydrogenated carbon (a:HC). The role of the carbon coating is twofold. It serves as a hard protection against friction and wear, and, because magnetic metals form strong chemical bonds with carbon, it protects the underlying magnetic substrate from corroding. In addition, a thin lubricant film (about 3 nm) is placed on top of the carbon overcoat. Increased storage capacity requires minimizing or possibly eliminating these coatings.

Researchers Jim Belak and Jim Glosli at LLNL and Michael Philpott at IBM are using MD simulation codes developed at LLNL to study the coatings and how they are modified by the tribological processes at the head–disk





Hard coating (a:HC)

The surface of a hard disk is coated with an ultrathin layer of amorphous hydrogenated carbon (a:HC) and perfluoropolyether (PFPE) lubricant to prevent friction and wear. The average spacing between the read/write head, which is carried by a slider, and the spinning disk is about 75 nm in today's technology. The need for even smaller spacing is driving our quest for increased understanding of the friction and wear properties of the protective coatings. To gain such understanding, Laboratory researchers are collaborating with researchers at IBM's Almaden Research Center to develop a molecular dynamics model of the coatings. The two images show our models of the lubricant and hard coating before contact.

interface. They have improved on an empirical model—the bond-order model—of chemical bonding in carbon films. Using this model to simulate the deposition process, they find that carbon atoms in amorphous films have a variety of local environments. When the environment is like that of diamond, the films are compact and hard. In contrast, films created at low deposition energy contain micrographitic structures. These graphitic films are soft. For the first time, understanding the microstructure of amorphous carbon films is within reach. The evolution of this microstructure controls the friction and wear rate.

The lubricant molecules used at the head–disk interface are perfluoropolyethers (PFPEs), which present additional difficulties for modelers because no model of cohesion exists for these lubricants. We are developing one based on models used to study large biomolecules. Preliminary results show that such commercial lubricants (with a molecular weight in the range of 4000) undergo significant rearrangement in the time scale for a slider to move about 100 nm over a disk surface. This result indicates that relaxation processes in the lubricants at the head-disk interface can be studied using MD simulations.

The next goal of our joint research is to provide an understanding of the fundamental physical and chemical processes during sliding. Such work is aimed at helping the engineering of the next generation of high-capacity, hard-disk drives. The research could also lead to much larger projects involving many technologies, including surface chemistry and physics, magnetics, and materials fabrication.

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